

Quantum transitions driven by one-bond defects in quantum Ising rings

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We investigate quantum scaling phenomena driven by lower-dimensional defects in quantum Ising-like models. We consider quantum Ising rings in the presence of a bond defect. In the ordered phase, the system undergoes a quantum transition driven by the bond defect between a *magnet* phase, in which the gap decreases exponentially with increasing size, and a *kink* phase, in which the gap decreases instead with a power of the size. Close to the transition, the system shows a universal scaling behavior, which we characterize by computing, either analytically or numerically, scaling functions for the gap, the susceptibility, and the two-point correlation function. We discuss the implications of these results for the nonequilibrium dynamics in the presence of a slowly-varying parallel magnetic field h , when going across the first-order quantum transition at $h = 0$.

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Quantum phase transitions [1] are phenomena of great interest in many different branches of physics. They arise in many-body systems in the presence of competing ground states. The driving parameters of the transition are usually bulk quantities, such as the chemical potential in particle systems, or external magnetic fields in spin systems. In the presence of first-order transitions, bulk behavior is particularly sensitive to the boundary conditions or to localized defects, hence it is possible to induce a quantum critical transition by changing only the parameters associated with the defects or the boundaries.

In this paper, we discuss an example of this type of transitions, considering a quantum Ising ring in a transverse magnetic field with a bond defect. In the ordered phase, bulk behavior of the low-energy states depends on the defect coupling. One may have a *magnet* phase, in which the gap decreases exponentially, i.e., $\Delta_L \sim e^{-cL}$ with increasing the size L , or a *kink* phase, in which the lowest states are one-kink states and $\Delta_L \sim 1/L^p$. Here, we analyze the crossover region between these phases, showing the emergence of a universal scaling behavior controlled by the defect coupling. We also analyze the slow nonequilibrium adiabatic dynamics [2, 3] across this transition. We obtain general time-dependent scaling laws that generalize to the first-order transition case those that characterize the Kibble-Zurek (KZ) mechanism at continuous transitions [3–5].

We consider Ising rings of size $L = 2\ell + 1$ in the presence of a transverse magnetic field and of one bond defect:

$$H_r = -J \sum_{i=-\ell}^{\ell-1} \sigma_i^{(1)} \sigma_{i+1}^{(1)} - g \sum_{i=-\ell}^{\ell} \sigma_i^{(3)} - \zeta \sigma_{-\ell}^{(1)} \sigma_{\ell}^{(1)}, \quad (1)$$

where $\sigma_i^{(a)}$ are the Pauli matrices. We set $J = 1$, and assume $g \geq 0$. Note that periodic (PBC), open (OBC), and antiperiodic (ABC) boundary conditions are recovered for $\zeta = 1, 0$, and -1 , respectively. The bond defect generally breaks translation invariance, unless $\zeta = \pm 1$.

A continuous transition occurs at $g = 1$, separating a disordered ($g > 1$) from an ordered ($g < 1$) phase [1]. In the presence of an additional parallel magnetic field h coupled to $\sigma_i^{(1)}$, a first-order quantum transition (FOQT) occurs at $h = 0$ for any $g < 1$, hence we expect the defect to be able to change bulk behavior for any $g < 1$. This is the regime we shall consider below.

Analytic and accurate numerical results can be obtained by exploiting the equivalent quadratic fermionic Hamiltonian which is obtained by a Jordan-Wigner transformation [6, 7]. We analyze the dependence of low-energy properties on the defect parameter ζ [8]. In particular, we consider the energy differences

$$\Delta_{L,n} \equiv E_n - E_0, \quad \Delta_L \equiv \Delta_{L,1}, \quad (2)$$

where E_0 is the energy of the ground state, and $E_{n \geq 1}$ are the (ordered) energies of the excited levels. The magnetization $\langle \sigma_x^{(1)} \rangle$ vanishes due to the global \mathbb{Z}_2 symmetry. Thus, we use the two-point correlation function $G(x, y) \equiv \langle \sigma_x^{(1)} \sigma_y^{(1)} \rangle$ to characterize the magnetic properties of the ground state.

For $g < 1$, we should distinguish a *magnet* phase ($\zeta > -1$) and a *kink* phase ($\zeta \leq -1$). The lowest states of the magnet phase are superpositions of states with opposite nonzero magnetization $\langle \pm | \sigma_x^{(1)} | \pm \rangle = \pm m_0$ (neglecting local effects at the defect), where [9] $m_0 = (1 - g^2)^{1/8}$. For a finite chain, tunneling effects between the states $|+\rangle$ and $|-\rangle$ lift the degeneracy, giving rise to an exponentially small gap Δ_L [10, 11]. For example, [9] $\Delta_L \approx 2(1 - g^2)g^L$ for $\zeta = 0$ (OBC). An analytic calculation gives

$$\Delta_L \approx \frac{8g}{1-g} w^2 e^{-wL}, \quad w = \frac{1-g}{g} (1 + \zeta), \quad (3)$$

for $\zeta \rightarrow -1^+$. The large- L two-point function is trivial,

$$G_r(x_1, x_2) \equiv \frac{G(x_1, x_2)}{m_0^2} \rightarrow 1 \quad (4)$$

for $x_1 \neq x_2$, keeping $X_i \equiv x_i/\ell$ fixed (but $X_i \neq \pm 1$).

The low-energy behavior drastically changes for $\zeta \leq -1$, in which the low-energy states are one-kink states (made of a nearest-neighbor pair of antiparallel spins), which behave as one-particle states with $O(L^{-1})$ momenta [1]. In particular, for $\zeta = -1$ (ABC) we have

$$\Delta_L = \frac{g}{1-g} \frac{\pi^2}{L^2} + O(L^{-4}). \quad (5)$$

The first two excited states are degenerate, thus $\Delta_{L,2} = \Delta_{L,1} \equiv \Delta_L$. For $\zeta < -1$, the ground state and the first excited state are superpositions with definite parity of the lowest kink $|\downarrow\uparrow\rangle$ and antikink $|\uparrow\downarrow\rangle$ states. The gap scales as [11, 12] L^{-3} ; we obtain explicitly

$$\Delta_L = \frac{8\zeta g^2}{(1-\zeta^2)(1-g)^2} \frac{\pi^2}{L^3} + O(L^{-4}). \quad (6)$$

On the other hand, $\Delta_{L,n}$ for $n \geq 2$ behaves as L^{-2} , e.g.,

$$\Delta_{L,2} = \frac{3g}{(1-g)} \frac{\pi^2}{L^2} + \frac{6(1-\zeta)g^2}{(1+\zeta)(1-g)^2} \frac{\pi^2}{L^3} + O(L^{-4}). \quad (7)$$

The two-point function $G(x, y)$ can be perturbatively computed for small g , obtaining the asymptotic large- L behaviors

$$G(x_1, x_2) = 1 - |X_1 - X_2| \quad \text{for } \zeta = -1, \quad (8)$$

$$G(x_1, x_2) = 1 - |X_1 - X_2| - \frac{|\sin(\pi X_1) - \sin(\pi X_2)|}{\pi} \quad (9)$$

for $\zeta < -1$, where $X_i \equiv x_i/\ell$. We conjecture (and verify numerically) that the above formulas can be straightforwardly generalized to the whole ordered phase $g < 1$ by simply introducing a multiplicative renormalization, i.e., by replacing G with $G_r \equiv G/m_0^2$.

These results suggest that $\zeta_c = -1$ is a critical point, separating the magnet and kink phases. We now show that around ζ_c the system develops a universal scaling behavior. We analytically compute (and verify numerically) the asymptotic behavior of $\Delta_{L,n}(\zeta)$, obtaining the scaling behavior

$$\Delta_{L,n}(\zeta) \approx \Delta_L(\zeta_c) D_n(\zeta_s), \quad (10)$$

$$\zeta_s = \frac{1-g}{g}(\zeta - \zeta_c) L, \quad \zeta_c = -1, \quad (11)$$

for $L \rightarrow \infty$ keeping the scaling variable ζ_s fixed. The scaling functions D_1 and D_2 are shown in Fig. 1 [13]. The cusp-like behavior at $\zeta_s = 0$ is the consequence of the crossing of the first two excited states at $\zeta = -1$. Generally, the scaling functions are universal apart from normalizations of their arguments. In this case, the normalization of ζ_s is chosen so that the scaling curves for different values of g are identical. Notice that, once the normalization is fixed by using one observable, universality should hold for any other observable. Numerical results for the energy differences $\Delta_{L,n}$ are shown in Fig. 1:

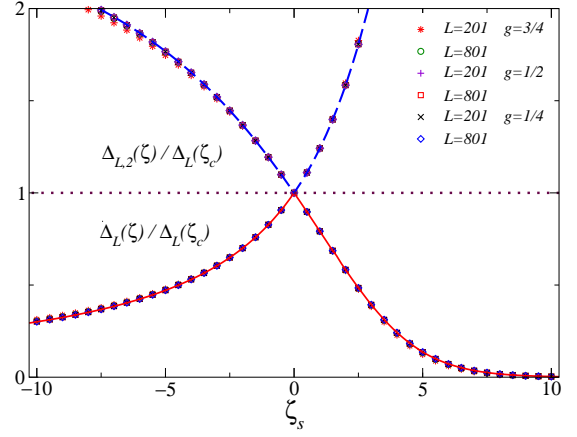


FIG. 1: (Color online) We show the scaling functions $D_n(\zeta_s)$, cf. Eq. (10), and numerical data for the ratio $\Delta_{L,n}(\zeta)/\Delta_L(\zeta_c)$, for $n = 1$ (bottom) and $n = 2$ (top) separated by the dotted line. Numerical data clearly approach the g -independent scaling curves $D_n(\zeta_s)$ (differences are hardly visible).

they confirm the scaling behavior (10). The asymptotic large- L behavior is generally approached with corrections of order L^{-1} .

Other observables satisfy analogous scaling relations. The two-point function is expected to behave as

$$G(x_1, x_2; \zeta) \approx m_0^2 \mathcal{G}(X_1, X_2; \zeta_s), \quad X_i = x_i/\ell, \quad (12)$$

where $m_0 = (1 - g^2)^{1/8}$. This scaling ansatz can be checked by considering the zero-momentum quantities

$$\chi = \sum_x G(0, x), \quad \xi^2 = \frac{1}{2\chi} \sum_x x^2 G(0, x) \quad (13)$$

(ξ is the second-moment length scale). Eq. (12) implies

$$\chi/L \approx m_0^2 f_\chi(\zeta_s), \quad \xi/L \approx f_\xi(\zeta_s). \quad (14)$$

Numerical data confirm them, see Fig. 2. In the language of renormalization-group (RG) theory, the defect coupling ζ plays the role of a relevant parameter at the magnet-kink transition, with RG dimension $y_\zeta = 1$.

An interesting question is whether there is a quantity playing the role of order parameter for the magnet-kink transition. This is provided by the center-defect correlation $b = \lim_{L \rightarrow \infty} G(0, \ell)$. Indeed, $b > 0$ for $\zeta > \zeta_c$ and $b = 0$ for $\zeta \leq \zeta_c$. Moreover, we observe the scaling behavior [14] $G(0, \ell) \sim L^{-1} f_b(\zeta_s)$, with $f_b(-\infty) = 0$ and $f_b(\infty) = \infty$, see Fig. 3.

An analogous magnet-to-kink quantum transition can be observed in the Ising chain by appropriately tuning a magnetic field η , coupled to $\sigma^{(1)}$, localized at the boundaries. Explicitly, we consider (we assume $\eta \geq 0$)

$$H_c = - \sum_{i=-\ell}^{\ell-1} \sigma_i^{(1)} \sigma_{i+1}^{(1)} - g \sum_{i=-\ell}^{\ell} \sigma_i^{(3)} - \eta (\sigma_{-\ell}^{(1)} - \sigma_{\ell}^{(1)}). \quad (15)$$

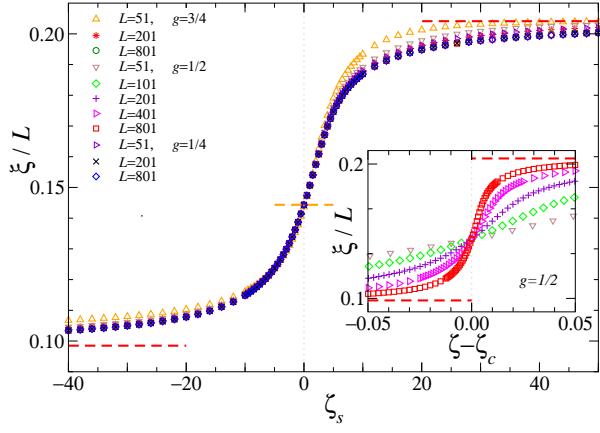


FIG. 2: (Color online) Estimates of the ratio ξ/L , supporting the scaling ansatz (14). Scaling corrections are only visible for $L \lesssim 100$. The dashed lines indicate the values of $f_\xi(\zeta_s)$ for $\zeta_s \rightarrow \pm\infty$ and $\zeta_s = 0$, obtained by matching the scaling ansatz with the behaviors in the different phases: $f_\xi(\infty) = 1/\sqrt{24}$ from Eq. (4), $f_\xi(-\infty) \approx 0.098491$ from Eq. (9), and $f_\xi(0) = 1/\sqrt{48}$ from Eq. (8). The inset shows the crossing point of data for different L implied by Eq. (14).

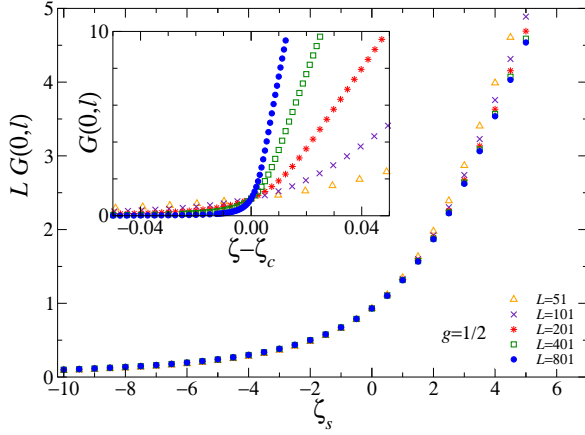


FIG. 3: (Color online) Scaling behavior of the center-defect correlation $G(0, \ell)$. The data of $LG(0, \ell)$ approach a scaling function of ζ_s . The inset shows $G(0, \ell)$ as a function of $\zeta - \zeta_c$.

The analytic computation of the low-energy spectrum identifies a particular value of the boundary field, $\eta_c = \sqrt{1-g}$, separating the magnet and kink phases. In the magnet phase $\eta < \eta_c$ we have

$$\Delta_L = \frac{2gs\sqrt{s^2-1}}{s-g} s^{-L} + O(s^{-2L}), \quad s = \frac{1-\eta^2}{g}. \quad (16)$$

For $\eta \geq \eta_c$ we have instead

$$\Delta_L = c(\eta) \frac{g}{1-g} \frac{\pi^2}{L^2} + O(L^{-3}) \quad (17)$$

with $c = 1$ for $\eta = \eta_c$ and $c = 3$ for any $\eta > \eta_c$. The similar nature of the coexisting phases suggests that their asymptotic large- L scaling behavior for $\zeta \approx \zeta_c$ and $\eta \approx$

η_c is the same, i.e., the two transitions belong to the same universality class. This is confirmed by analytic and numerical computations, although the comparison of the results is not straightforward, as the Ising chain (15) breaks the \mathbb{Z}_2 symmetry, which is instead preserved by the Ising ring (1). For example, the gap satisfies scaling relations analogous to Eq. (10). Explicitly,

$$\Delta_{L,n}(\eta) = \Delta_L(\eta_c) E_n(\eta_s), \quad \eta_s = \frac{2\sqrt{1-g}}{g} (\eta_c - \eta)L, \quad (18)$$

with [15] $E_n(x) = D_{2n-1}(x)$ for $x \geq 0$ and $E_n(x) = D_{2n}(x)$ for $x \leq 0$. The reason of the peculiar mapping is related to the different behavior under \mathbb{Z}_2 of the two models. Consider for instance the kink phase. While in the Ising ring the lowest states are superpositions of kink and antikink configurations, in the case of model (15) the parity symmetry is broken by the boundary fields, thus only kink states are left. Hence, model (15) has only half of the states of the Ising ring. Moreover, no degeneracy occurs at $\eta = \eta_c$ so that levels must be smooth at the transition point, thereby explaining why the mapping between the levels must change at the transition point (in the ring case, cusps occur at the transition).

It is worth noting that, at the critical value $g = 1$, corresponding to the order-disorder continuous transition, bulk behavior is independent of the boundary conditions or of the presence of defects, hence the magnet-to-kink transition only occurs for g strictly less than 1. For instance, the gap at $g = 1$ behaves as $\Delta_L \sim L^{-1}$ for any ζ or η . Of course, the prefactor depends on the boundary conditions; see, e.g., the known results for PBC, OBC, and ABC, summarized in Ref. [16].

It is interesting to reinterpret our results in the equivalent fermionic picture of models (1) and (15). In the magnet phase, i.e., for $\zeta > \zeta_c$ and $\eta < \eta_c$, respectively, the lowest eigenstates are superpositions of Majorana fermionic states localized at the boundaries or on the defect [17, 18]. In finite systems, their overlap does not vanish, giving rise to the splitting $\Delta \sim e^{-L/l_0}$. The coherence length l_0 diverges at the kink-to-magnet transitions as $l_0^{-1} \sim |\ln s| \sim \eta_c - \eta$ and $l_0^{-1} \sim \zeta - \zeta_c$ in the two models, a behavior analogous to that observed at the order-disorder transition $g \rightarrow 1^-$ where $l_0^{-1} \sim |\ln g|$.

In conclusion, we have shown that quantum transitions can be induced by tuning the boundary conditions or by changing lower-dimensional defect parameters, when the system is at a FOQT. We have explicitly discussed this behavior in the case of quantum Ising rings in a transverse field. If $g < 1$, this model shows a magnet and a kink phase, separated by a quantum transition point. In its neighborhood, we can define general scaling laws, that are analogous to those that hold at continuous transitions. The same scaling behavior is also observed in the XY quantum ring in which one adds additional bond couplings $\sigma_i^{(2)} \sigma_{i+1}^{(2)}$ [19], and in the quantum Ising chain

with opposite magnetic fields at the boundaries. The universal scaling behavior is essentially the same and is uniquely determined by the structure of the low-energy behavior in the two phases. We have characterized the scaling variable and computed the scaling functions of different observables. These scaling behaviors can be straightforwardly extended to allow for a nonzero temperature T , by considering a further dependence on the scaling variable $TL^z = TL^2$. Even though we have discussed the issue in one dimension, we expect the same type of behavior in quantum d -dimensional Ising models defined in $L^{d-1} \times M$ boxes with $L \gg M$, in the presence of a $(d-1)$ -dimensional surface of defects or of opposite magnetic fields on the L^{d-1} boundaries.

The size dependence of the low-energy spectrum is relevant for the understanding of the nonequilibrium unitary dynamics, as it determines the conditions for a nearly adiabatic quantum dynamics [2, 3]. Significantly different behaviors are expected in the magnet and kink phases when we add a time-dependent parallel magnetic term,

$$H_t = H - h(t/t_0) \sum_i \sigma_i^{(1)}, \quad h(u) = h_0 u, \quad (19)$$

where t_0 is the time scale of the time dependence. Adiabatic evolutions across the FOQT ($h(0) = 0$) require very different time scales t_0 . In the magnet phase we must have $t_0 \gtrsim e^{2L/l_0}$, while in the kink phase $t_0 \gtrsim L^4$ at ζ_c (η_c) and $t_0 \gtrsim L^6$ for $\zeta < \zeta_c$ [$t_0 \gtrsim L^4$ for $\eta > \eta_c$ in model (15)]. The dynamics in the magnet phase is essentially equivalent to that of a two-level Landau-Zener model with an exponentially small gap [20, 21]. At ζ_c for model (1) and $\eta \geq \eta_c$ for model (15), dynamics becomes similar to that at a continuous transition with a dynamic exponent $z = 2$, since there is a tower of excited states with $\Delta_{L,n} = O(L^{-2})$. Model (1) for $\zeta < \zeta_c$ shows again a low-energy dynamics dominated by the two lowest states with a gap of order L^{-3} . The above results suggest that nonequilibrium scaling laws, such as those describing the KZ mechanism at continuous transitions [3–5] (when systems are ramped across a continuous transition at a finite rate), also hold at FOQTs, when the time-dependent h crosses the value $h = 0$. The slow nonequilibrium dynamics of the Hamiltonian (19) across the FOQT $h = 0$, and in particular the interplay among t , t_0 , ζ (or η) and L , thus Δ_L , can be described by a scaling theory which extends the equilibrium scaling behaviors (12) and (14). For this purpose, we use scaling arguments similar to those employed to describe the KZ problem [5]. If $y_h = d + z$ (d is the space dimension, $d = 1$ in our example) is the effective RG dimension of the parallel field h ($z = 2$ and $y_h = 3$ in the Ising chain [22]), we can define an effective length scale ξ_h associated with h that scales as $\xi_h \sim h^{-1/y_h}$. The dynamical scaling laws for a system of size L can be heuristically derived by substituting h with the time-dependent $h(t/t_0)$ into the scaling combinations $t\xi_h^{-z} = th^{z/y_h}$ and ξ_h/L . This gives $t(t/t_0)^{z/y_h} =$

$(t/\tau)^{1+z/y_h}$ and $L/\xi_h = L(t/t_0)^{1/y_h} = (t/\tau)^{1/y_h} L/\tau^{1/z}$, with $\tau = t_0^{z/(z+y_h)} = t_0^{2/5}$ [23]. These considerations lead us to conjecture the scaling behavior for the Ising chain

$$\langle \sigma_x^{(1)} \rangle \approx m_0 f_m(x/L, t/\tau, \tau/L^2, \zeta_s), \quad (20)$$

$$\langle \sigma_{x_1}^{(1)} \sigma_{x_2}^{(1)} \rangle \approx m_0^2 f_g(x_i/L, t/\tau, \tau/L^2, \zeta_s), \quad (21)$$

with ζ_s given by Eq. (11). Analogous expressions apply to other observables and to the model (15). Of course, the above nonequilibrium scaling theory should be further investigated, to get a thorough understanding of KZ-like phenomena at FOQTs.

These issues may also be relevant in the context of quantum computing. Adiabatic algorithms rely on sufficiently large gaps during the variation of the model parameters bringing to the ground state of the desired Hamiltonian [24–26]. Thus, FOQTs, at which the gap is exponentially small, represent a hard problem [27–29]. As a simple paradigmatic case we may consider the time-dependent Hamiltonian (19) for $g < 1$ and $\zeta = 1$. Let us assume that we want to adiabatically move from the ground state with $h = -h_0$ at time $t = -T_a$ to the ground state with $h = h_0$ at $t = T_a$. This requires an exponentially large time scale, i.e. $T_a \gtrsim e^{2L/l_0}$. Our results for the ζ -dependence of the low-energy properties suggest a way to overcome this hard problem. Indeed, instead of changing directly h , one could proceed as follows. First, one adiabatically changes the system varying the bond defect from $\zeta = 1$ to $\zeta \lesssim \zeta_c$, which corresponds to adding a further single-bond Hamiltonian term $H_\zeta = -\zeta(t/T_\zeta) \sigma_{-\ell}^{(1)} \sigma_\ell^{(1)}$. In the presence of a finite parallel magnetic field $h = -h_0$, the gap is finite. Then, one adiabatically changes h , according to Eq. (19), which now requires a time scale $T_a \gtrsim L^4$ or L^6 to adiabatically go from $-h_0$ to h_0 . Finally, ζ is increased again to $\zeta = 1$, obtaining the ground state of the original problem in a total time that scales with a power, and not with the exponential, of the size. Therefore, by taking advantage of particular sensitivity of FOQTs to defects or boundary perturbations, one may overcome the problem of an exponentially slow dynamics, which occurs at FOQTs within the more standard approaches.

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